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PSEUDOPOTENTIALS AND STRUCTURE-PROPERTY RELATIONSHIPS
IN THE SOLID STATE(U) CHICAGO UNIV IL DEPT OF CHEMISTRY
J K BURDETT 01 APR 86 N00014-85-K-0354

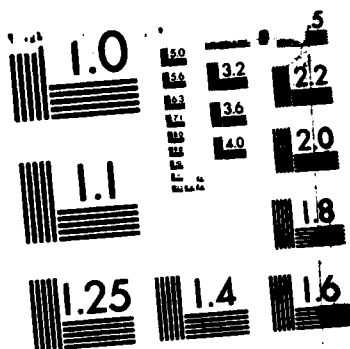
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The dielectric theory of Phillips and Van Vechten defines crystalline ionicity in terms of optical properties and predicts first-order structural phase transitions. Their approach, while very successful, is, nonetheless, empirical and has yet to be justified via an ab initio quantum mechanical approach. We present such an approach for examining the relationship between spectroscopic crystal ionicity and spatial structure. We demonstrate that the structural predictions based on ionicity scales derived from the dielectric theory are consistent with a microscopic point of view.

Pseudopotential radii are used to sort ternary systems. By and large the sorting is only slightly better than that found using ionic radii, although the use of a third parameter allows sorting of the spinel and Cr_3S_4 types.

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This annual report covers the period from April 15, 1985 to April 14, 1986. The report includes two technical reports on completed work which are being sent out to those on the distribution list as required.

The numerical work during the year has concentrated on two aspects of solids (i) seeing how well the pseudopotential approach developed by Chelikowsky and Louie works in getting the correct structure for simple solids and trying to understand why, as one moves across a pseudopotential structure map the stable structure changes. This work has now been published as a Physical Review Letter (Technical Report #1), (ii) Examination of the electronic band structures of some simple solids using less accurate methods in order to see how the substitution of Si for P or P for S in binary or ternary systems changes the details of the electronic structure and the relevant bond gaps. This work is in progress and represents the introduction to the solid state for a new postdoctoral.

In qualitative terms we have used the aspects of pseudopotential radii to plot structure maps for ternary materials. Their use does allow a superior sorting compared to the ionic radii but is not particularly startling (Technical Report #2). We have had less success in correlating properties with the pseudopotential radii due entirely to the lack of a sufficiently large database of properties.

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